Spin-Peierls Dimerization of a $s = \frac{1}{2}$ Heisenberg Antiferromagnet on a Square Lattice

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Abstract

Dimerization of a spin-half Heisenberg antiferromagnet on a square lattice is investigated for several possible dimerized configurations, some of which are shown to have lower ground state energies than the others. In particular, the lattice deformations resulting in alternate stronger and weaker couplings along both the principal axes of a square lattice are shown to result in a larger gain in magnetic energy. In addition, a 'columnar' configuration is shown to have a lower ground state energy and a faster increase in the energy gap parameter than a 'staggered' configuration. The inclusion of unexpanded exchange coupling leads to a power law behaviour for the magnetic energy gain and energy gap, which is qualitatively different from that reported earlier. Instead of increasing as δ^x, the two quantities depend on δ as $\delta^\nu / |\ln \delta|$. This is true both in the near critical regime ($0 \le \delta \le 0.1$) as well as in the far regime ($0 \le \delta < 1$). It is suggested that the unexpanded exchange coupling is as much a source of the logarithmic dependence as a correction due to the contribution of umklapp processes. Staggered magnetization is shown to follow the same δ-dependence in all the configurations in the small δ-regime, while for $0 \le \delta < 1$, it follows the power law δ^x.

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I. INTRODUCTION

It is known that dimerization lowers the ground state energy of a spin-half isotropic Heisenberg antiferromagnet [1–10]. In other words, the system stands to gain energy by such lattice deformations that render it dimerized with alternate weaker and stronger bonds between spins on neighboring sites. On the other hand the lattice distortions cost energy and it is the net energy balance that would determine whether the gain in magnetic energy $\varepsilon(\delta) - \varepsilon(0)$ is large enough to affect the spin-Peierls transition through dimerization. In a phenomenological theory, this is usually seen in terms of an exponent showing the dependence of magnetic and elastic energies on the dimerization parameter δ; where $0 \le \delta < 1$. The parameter δ describes the extent of lattice deformation, i.e., it gives the displacement of the ith atom through $u_i = \frac{1}{2}(-1)^i \delta$. The spin-dimer formation is usually described by the Hamiltonian

$$H = J \sum_i [1 + (-1)^i \delta] \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{1}$$

envisaging alternate stronger and weaker exchange bonds $J(1 + \delta)$ and $J(1 - \delta)$. These bonds can, in fact, be seen to result from the ansatz $J(a) = \frac{J}{a}$ [11]. Thus when the distance between a pair of spins decreases from a to $a(1 - \delta)$, the exchange coupling is taken to change from J to approximately $J(1 + \delta)$.

1

Since $0 \leq \delta \leq 1$, and since elastic energies go typically as δ^2, therefore if the magnetic energy gain varies with δ with an exponent less than 2 then in the limit $\delta \to 0$, the gain would overwhelm the cost. In situations where the ground state is amenable to dimerization, the spin-Peierls transition will be unconditional [9,12].

Such aspects as these have been studied extensively in Heisenberg antiferromagnetic chains, as summarized in Table 1. This aspect has also been revealed by experiments on quasi-one dimensional Heisenberg antiferromagnet $CuGeO_3$ [13–15].

The situation in two-dimensions is a little more involved because of the possibility of frustration due to a competing antiferromagnetic second neighbour interaction which can in principle destroy any LRO of the Neel type as well as the possibility of dimerization. Much of the study of two-dimensional Heisenberg antiferromagnet has therefore remained focused on the destruction of order by frustration [16]. Moreover, the ground state of a Heisenberg antiferromagnet on a square lattice at zero temperature is Neel-ordered and a critical value of spin-lattice coupling is required for the gain in magnetic energy to affect a spin-Peierls transition [12,17,18]. It is assumed below that the spin-lattice coupling is above the threshold, allowing for dimerization of the lattice. The spin configuration is expected to remain Neel-like under dimerization. This is true in the absence of either frustration or quantum fluctuations which lead to a melting of the Neel lattice [19].

The matter of frustration and quantum fluctuation aside, a simple dimerization of a square lattice is interesting in its own right because the lattice distortions can take place in more than one way, each one of the possible configurations giving a different dependence of the ground state energy on the dimerization parameter.

Figure (1) shows a few such configurations. Fig.(a) describes a columnar configuration caused by one longitudinal static $(\pi, 0)$ phonon, in which the nearest neighbour distances along the x-axis are taken to vary alternately as $a(1+\delta)$, while those along the y-direction remain a. Fig.(b) shows a staggered configuration in which the lattice deformation along the x-direction is alternated as in Fig.(a), but the sequence of alternations is itself alternated as one goes along the y-direction. It is caused by a (π, π) phonon with polarization along the x-axis [12]. The difference between the earlier considerations of this configuration and ours is that we take into account the elongation in the exchange bond along the y-direction also, making it dependent upon the dimerization parameter δ. While the coupling along the x-direction is alternately $\frac{J}{1-\delta}$ and $\frac{J}{1+\delta}$, it is uniformly $\frac{J}{\sqrt{(1+\delta^2)}}$ along the y-direction.

In contrast to the configurations (a) and (b), those in Figs.(c), (d) and (e) allow for simultaneous dimerization along both x- and y-directions in the plane. The difference between (c) and (d) is the same as that between (a) and (b): configuration (c) is columnar and (d) is staggered. The former, caused by two phonons with wavevectors $(\pi, 0)$ and $(0, \pi)$, is called plaquette configuration [12,20]. Fig.(e) shows a much studied configuration, caused by a longitudinal (π, π) phonon mode. In these three configurations also the exchange couplings in both $x-$ and $y-$ directions are δ-dependent. These five configurations of a dimerized square lattice consisting of N spins are therefore characterized by the following nearest neighbour interactions.

Configuration (a)

$J_{x,\lambda} = \frac{J}{(1+\lambda\delta)} \simeq J(1 - \lambda\delta), \lambda = \pm 1$
$J_y = J.$

That is to say, the dimerization is described by the Hamiltonian

$$H = J \sum_{i,j}^{\sqrt{N}} \left[\frac{1}{(1 + (-1)^i \delta)} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} \right] \tag{2}$$

Configuration (b)

$J_{x,\lambda} = \frac{J}{(1+\lambda\delta)} \simeq J(1 - \lambda\delta), \lambda = \pm 1$
$J_y = \frac{J}{\sqrt{1+\delta^2}} \simeq J(1 - \frac{\delta^2}{2})$

and the Hamiltonian is given by

$$H = J \sum_{i,j}^{\sqrt{N}} \left[\frac{1}{(1+(-1)^{i+j}\delta)} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + \frac{1}{\sqrt{1+\delta^2}} \; \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} \right]. \tag{3}$$

Configuration (c)

$J_{x,\lambda} = J_{y,\lambda} = \frac{J}{(1+\lambda\delta)} \simeq J(1-\lambda\delta), \; \lambda = \pm 1$

with the Hamiltonian

$$H = J \sum_{i,j}^{\sqrt{N}} \left[\frac{1}{(1+(-1)^i\delta)} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + \frac{1}{(1+(-1)^j\delta)} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} \right]. \tag{4}$$

Configuration (d)

$J_{x,\lambda} = \frac{J}{(1+\lambda\delta)} \simeq J(1-\lambda\delta), \; \lambda = \pm 1$

$J_{y,\lambda} = \frac{J}{\sqrt{\delta^2+(1+\lambda\delta)^2}} \simeq J\left(1-\lambda\delta-(1-\frac{\lambda^2}{2})\delta^2\right)$

and the Hamiltonian

$$H = J \sum_{i,j}^{\sqrt{N}} \left[\frac{1}{(1+(-1)^{i+j}\delta)} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + \frac{1}{\sqrt{\delta^2 + (1+(-1)^j\delta)^2}} \; \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} \right]. \tag{5}$$

Configuration (e)

$J_{x,\lambda} = J_{y,\lambda} = \frac{J}{\sqrt{\delta^2+(1+\lambda\delta)^2}} \simeq J\left(1-\lambda\delta-(1-\frac{\lambda^2}{2})\delta^2\right), \; \lambda = \pm 1$

and the Hamiltonian

$$H = J \sum_{i,j}^{\sqrt{N}} \frac{1}{\sqrt{\delta^2 + (1+(-1)^{i+j}\delta)^2}} \left[\mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} \right]. \tag{6}$$

Some of the exchange couplings in Eqs.(2-6) blow up at $\delta = 1$. Our analysis will therefore be confined to $0 \le \delta < 1$.

We would like to investigate the five configurations in order to see (i) which of them gives the largest gain in magnetic energy as the dimerization sets in, and (ii) whether the use of untruncated exchange coupling leads to a single power law valid for the entire range of δ.

A number of methods can be chosen for this purpose. Spin wave theory, either modified through Takahashi constraint of zero magnetization or a Hartree-Fock approximated non-linear theory, is known to give surprisingly good results for spin-half Heisenberg antiferromagnet. Or, a spin wave theory in the spinless fermionic representation through Jordan-Wigner transformations takes care of fermionic correlations among the $s = \frac{1}{2}$ spins. Coupled cluster method (CCM) has also been extensively, and successfully, used for spin-half Heisenberg antiferromagnet in one and two space dimensions.

The first two methods belong to the class of mean field theories and hence are not expected to be very reliable when it comes to determining critical exponents. The coupled cluster method, on the other hand, is a perturbation method in which increasingly higher order correlations can, in principle, be incorporated at will, and which has been shown to give satisfactory results even in the lower orders of perturbation [21,22]. We believe that the coupled cluster method must be sufficiently good to see which of the alternative configurations proposed here is favoured once a spin-Peierls transition sets in.

II. APPLICATION OF THE COUPLED-CLUSTER METHOD

In the coupled cluster method it is first necessary to define a ket state starting from a model state $| \phi >$, which in our case is the Neel state. The exact ground state $| \Psi >$ of the system can then be postulated as

$$| \Psi >= e^{\mathcal{S}} | \phi > \tag{7}$$

where $\mathcal{S}$ is the correlation operator defined for an N particle system as

$$\mathcal{S} = \sum_n \mathcal{S}_n \tag{8}$$

$$\text{with } \mathcal{S}_n = \sum_{i_1 \ldots i_n} \mathsf{S}_{i_1, \ldots, i_n} C^{\dagger}_{i_1} C^{\dagger}_{i_2} \cdots \cdots C^{\dagger}_{i_n} \tag{9}$$

and $C^{\dagger}_i$ is the creation operator defined with respect to the model state. The ground state energy can then be found as the eigenvalue of the Hamiltonian in the proposed ground state

$$H e^{\mathcal{S}} | \phi >= E_g e^{\mathcal{S}} | \phi >.$$

Taking inner product with $< \phi | e^{-\mathcal{S}}$ gives

$$E_g =< \phi | e^{-\mathcal{S}} H e^{\mathcal{S}} | \phi > .$$

The product $e^{-\mathcal{S}} H e^{\mathcal{S}}$ can be written as a series of nested commutators in the well-known expansion

$$e^{-\mathcal{S}} H e^{\mathcal{S}} = H + [H, \mathcal{S}] + \frac{1}{2!} [[H, \mathcal{S}], \mathcal{S}] + \cdots\cdots\cdots \tag{10}$$

where in the present case the series terminates after the fourth term.

It is usually easier to deal with the $s = \frac{1}{2}$ Heisenberg Hamiltonian by applying a rotation of $180°$ to the up spin sublattice; $S_x \rightarrow -S_x$, $S_y \rightarrow S_y$ and $S_z \rightarrow -S_z$ such that all the spins in the lattice point down. It is also convenient to replace the spin operators with Pauli matrices: $S^j = \frac{1}{2}\sigma^j$, $j = x, y, z$ [21,22]. A general expression for the nearest neighbour spin Hamiltonian in 2D is then

$$H = -\frac{J}{4} \sum_{\mathbf{l}, \rho} \left(2(\sigma^+_{\mathbf{l}} \sigma^+_{\mathbf{l}+\rho} + \sigma^-_{\mathbf{l}} \sigma^-_{\mathbf{l}+\rho}) + \sigma^z_{\mathbf{l}} \sigma^z_{\mathbf{l}+\rho} \right), \tag{11}$$

where ρ is a vector to the four nearest neighbours. Correspondingly, the string operator $\mathcal{S}_n$ can now be defined as

$$\mathcal{S}_{2n} = \frac{1}{(n!)^2} \sum_{\mathbf{i}_1 \ldots \mathbf{i}_n} \sum_{\mathbf{j}_1 \ldots \mathbf{j}_n} \mathsf{S}_{\mathbf{i}_1 \ldots \mathbf{i}_n; \ \mathbf{j}_1 \ldots \mathbf{j}_n} \sigma^+_{\mathbf{i}_1} \sigma^+_{\mathbf{i}_2} \cdots \sigma^+_{\mathbf{i}_n} \sigma^+_{\mathbf{j}_1} \sigma^+_{\mathbf{j}_2} \cdots \sigma^+_{\mathbf{j}_n}, \tag{12}$$

where subscripts $\mathbf{i}$ and $\mathbf{j}$ distinguish between sites on the two sublattices. We note that for spin half $(\sigma^+_{\mathbf{l}})^2 = (\sigma^-_{\mathbf{l}})^2 = 0$. Truncation of the summation up to the desired level gives rise to different schemes of approximation. Taking interaction only between the spins on adjacent sites gives the so-called SUB$_{2-2}$ scheme. Including interactions with the second and fourth neighboring sites gives what is termed as SUB$_{2-4}$ scheme. And taking the previous two schemes including interaction among the four adjacent sites give us what has been termed as local SUB$_4$, or LSUB$_4$ for short. Each one of these approximations accounts for a different order of perturbation calculation, and takes into account a different order of inter-particle correlations. It has been noted that LSUB$_4$ is a sufficiently good approximation for calculating the ground state properties of a spin-half Heisenberg system [22].

Consider a general case: a Hamiltonian which has four different coupling constants for nearest neighbour interactions in two space dimensions. It can be written as

$$H = -\frac{1}{4} \sum_{i,j}^{\sqrt{N}/2} \sum_{\lambda=\pm 1} [J_{x,\lambda} \ \sigma_{2i,j} \cdot \sigma_{2i+\lambda,j} + J_{y,\lambda} \ \sigma_{i,2j} \cdot \sigma_{i,2j+\lambda}]. \tag{13}$$

4

Here i and j are the two components of the site indices on a square lattice. The correlation operators in the LSUB$_4$ scheme are defined as

$$S_2 = \sum_{i,j} \left[a_1 \; \sigma^+_{2i,j}\sigma^+_{2i+1,j} + b_1\sigma^+_{2i,j}\sigma^+_{2i-1,j} \; + c_1\sigma^+_{i,2j}\sigma^+_{i,2j+1} + d_1\sigma^+_{i,2j}\sigma^+_{i,2j-1} \right]$$

$$S_3 = \sum_{i,j} \left[a_3\sigma^+_{2i,j}\sigma^+_{2i+3,j} \; + b_3\sigma^+_{2i,j}\sigma^+_{2i-3,j} \; + c_3\sigma^+_{i,2j}\sigma^+_{i,2j+3} + d_3\sigma^+_{i,2j}\sigma^+_{i,2j-3} \right]$$

$$S_4 = \sum_{i,j} \left[f \prod_{\nu=0}^{3} \sigma^+_{2i+\nu,j} + g \prod_{\nu=0}^{3} \sigma^+_{2i-\nu,j} + h \prod_{\nu=0}^{3} \sigma^+_{i,2j+\nu} + l \prod_{\nu=0}^{3} \sigma^+_{i,2j-\nu} \right] \tag{14}$$

In these equations, the coefficients $a_1, b_1,$ etc., are various forms of the coefficient $S_{\mathbf{i_1}\ldots\mathbf{i_n}\,;\,\mathbf{j_1}\ldots\mathbf{j_n}}$ in the expressions for S_{2n}. The ground state energy within the LSUB$_4$ approximation comes out to be

$$E_g = -\frac{1}{16} \left[J_{x,+1} \; (1 + 4a_1) + J_{x,-1} \; (1 + 4b_1) + J_{y,+1} \; (1 + 4c_1) + J_{y,-1} \; (1 + 4d_1) \right] \tag{15}$$

The coefficients $a_1, a_2, \cdots, l$ are obtained as solutions of a set of coupled nonlinear equations. These equations arise from the fact that such matrix elements as $< \phi \mid \mathbf{O} \; e^{-S} H e^{S} \mid \phi >$ are all zero when the operator $\mathbf{O}$ is any product of creation operators, particularly if it is one of the operator products in the correlation operator S above.

$$\begin{aligned}
&< \sigma^-_{i,2j}\sigma^-_{i,2j+\nu} e^{-S} H e^{S} >= 0; & \nu = \pm 1, \pm 3 \\
&< \sigma^-_{2i,j}\sigma^-_{2i+\nu,j} e^{-S} H e^{S} >= 0; & \nu = \pm 1, \pm 3 \\
&< \sigma^-_{2i,j}\sigma^-_{2i+\nu,j}\sigma^-_{2i+2\nu,j}\sigma^-_{2i+3\nu,j} e^{-S} H e^{S} >= 0; & \nu = \pm 1 \\
&< \sigma^-_{i,2j}\sigma^-_{i,2j+\nu}\sigma^-_{i,2j+2\nu}\sigma^-_{i,j+3\nu} e^{-S} H e^{S} >= 0; & \nu = \pm 1
\end{aligned} \tag{16}$$

where $S = S_2 + S_3 + S_4$. These equations translate into the following twelve equations for the unknown parameters:

$$(a_1^2 - 1 - 2a_3 b_1 - 2f)J_{x,+1} + (2a_1 + 2a_1 b_1 - 2a_3 b_3)J_{x,-1} = 0$$

$$(2b_1 + 2a_1 b_1 - 2a_3 b_3)J_{x,+1} + (b_1^2 - 1 - 2a_1 b_3 - 2g)J_{x,-1} = 0$$

$$(2a_3 + 2a_1 a_3)J_{x,+1} + (2a_3 - a_1^2 + 2a_3 b_1 - f)J_{x,-1} = 0$$

$$(2b_3 - b_1^2 + 2a_1 b_3 - g)J_{x,+1} + (2b_3 + 2b_1 b_3)J_{x,-1} = 0$$

$$(-2a_3 b_1 + 2a_1 f + a_3 b_1^2 - a_1 a_3 b_1)J_{x,+1} + (f - a_1^2 + 2b_1 f + a_3 g + 2a_1 a_3 b_3)J_{x,-1} = 0$$

$$(g - b_1^2 + 2a_1 g + b_3 f + 2a_3 b_1 b_3)J_{x,+1} + (-2a_1 b_3 + 2b_1 g + a_1^2 b_3 - a_1 b_1 b_3)J_{x,-1} = 0$$

$$(c_1^2 - 1 - 2c_3 d_1 - 2h)J_{y,+1} + (2c_1 + 2c_1 d_1 - 2c_3 d_3)J_{y,-1} = 0$$

$$(2d_1 + 2c_1 d_1 - 2c_3 d_3)J_{y,+1} + (d_1^2 - 1 - 2c_1 d_3 - 2l)J_{y,-1} = 0$$

$$(2c_3 + 2c_1 c_3)J_{y,+1} + (2c_3 - c_1^2 + 2c_3 d_1 - h)J_{y,-1} = 0$$

$$(2d_3 - d_1^2 + 2c_1 d_3 - l)J_{y,+1} + (2d_3 + 2d_1 d_3)J_{y,-1} = 0$$

$$(-2c_3 d_1 + 2c_1 h + c_3 d_1^2 - c_1 c_3 d_1)J_{y,+1} + (h - c_1^2 + 2d_1 h + c_3 l + 2c_1 c_3 d_3)J_{y,-1} = 0$$

$$(l - d_1^2 + 2c_1 l + d_3 h + 2c_3 d_1 d_3)J_{y,+1} + (-2c_1 d_3 + 2d_1 l + c_1^2 d_3 - c_1 d_1 d_3)J_{y,-1} = 0$$

Setting all the coupling constants J_μ equal reduces the number of equations from twelve to three and yields exactly the same equations as obtained by others [21,22]. The two sets of six equations each independently determines the six coefficients contained in each of them. As expected, the equations are symmetric in some coefficients. The twelve coefficients are to be evaluated by solving the above coupled equations numerically for each of the configurations

separately by substituting appropriate values of $J_{x,\lambda}$ and $J_{y,\lambda}$.

To be able to calculate the energy gap between the ground and the first excited states, we shall construct the excited ket state $|\Psi_e>$ in term of a linear excitation operator $\mathbf{X}$, which, operating on the ground state $|\Psi_0>$, takes the system to an excited state: $|\Psi_e> = \mathbf{X} |\Psi_0> = \mathbf{X}e^{\mathcal{S}} |\phi>$. This operator is constructed as a linear combination of products of creation operators [22]

$$\mathbf{X} = \sum_n X_n \tag{17}$$

with

$$X_n = \sum_{\mathbf{j}_1,\dots,\mathbf{j}_n} \chi_{\mathbf{j}_1,\dots,\mathbf{j}_n} \sigma_{\mathbf{j}_1}^+ \sigma_{\mathbf{j}_2}^+ \cdots \sigma_{\mathbf{j}_n}^+. \tag{18}$$

The first excited state is obtained by the operator

$$X_1 = \sum_{\mathbf{j}} \chi_{\mathbf{j}} \sigma_{\mathbf{j}}^+ \tag{19}$$

where $\mathbf{j}$ can be any site of the two sublattices. It is easily seen that the first excitation energy is

$$E_e = \frac{1}{8}\left(\frac{1}{2} + 2a_1 + 2b_1 + 2a_3 + 2b_3\right)(J_{x,+1} + J_{x,-1}). \tag{20}$$

The energy gap for a given δ is $\Delta(\delta) = E_e(\delta) - |E_g(\delta)|$. We define gap parameter as $D(\delta) = \Delta(\delta) - \Delta(0)$. This is the energy required to break a dimerized singlet pair for a given δ.

To be able to calculate a quantity like staggered magnetization the need of defining the bra state arises. In fact the bra state is not simply a conjugate of the ket state defined in Eq.(7). The bra ground state wave function $< \widetilde{\Psi}|$ corresponding to the ket state $|\Psi>$ can be defined as [21,22]

$$< \widetilde{\Psi}| = < \phi| \, \widetilde{\mathcal{S}}_{2n}e^{-\mathcal{S}}$$

where the correlation operator $\widetilde{\mathcal{S}}$ is built wholly out of destruction operators of the Hamiltonian used. The need of defining such operators comes from the fact that $e^{-\mathcal{S}}$ is not equal to $e^{\mathcal{S}^\dagger}$. In our case the correlation operator is defines as

$$\widetilde{\mathcal{S}}_{2n} = 1 + \sum_{n=1}^{N/2} \widetilde{s}_{2n}$$

with

$$\widetilde{s}_{2n} = \frac{1}{(n!)^2} \sum_{\mathbf{i}_1,\dots,\mathbf{i}_n} \sum_{\mathbf{j}_1,\dots,\mathbf{j}_n} \widetilde{\mathsf{S}}_{\mathbf{i}_1\dots\mathbf{i}_n;\ \mathbf{j}_1,\dots,\mathbf{j}_n} \sigma_{\mathbf{i}_1}^- \sigma_{\mathbf{i}_2}^- \cdots \sigma_{\mathbf{i}_n}^- \sigma_{\mathbf{j}_1}^- \sigma_{\mathbf{j}_2}^- \cdots \sigma_{\mathbf{j}_n}^-,$$

where $\mathbf{i}$ and $\mathbf{j}$ indicate vectors in the two sublattices respectively. The first term in $\widetilde{\mathcal{S}}_{2n}$ ensures orthonormality of the bra and ket state; i.e., $< \widetilde{\Psi}|\Psi> \ = \ < \phi|\Psi> \ = \ < \phi|\phi> \ = 1$. The bra state coefficients are found by putting the matrix elements of the commutator of the Hamiltonian with a string of creation operators in the states $\widetilde{\Psi}$ and Ψ to zero.

$$< \phi| \, \widetilde{\mathcal{S}}e^{-\mathcal{S}}[H, \sigma_{\mathbf{i}_1}^+ \sigma_{\mathbf{i}_2}^+ \cdots \sigma_{\mathbf{i}_n}^+ \sigma_{\mathbf{j}_1}^+ \sigma_{\mathbf{j}_2}^+ \cdots \sigma_{\mathbf{j}_n}^+]e^{\mathcal{S}}|\phi> = 0, n = 1,2,3,\cdots \tag{21}$$

Equations(21) form a set of coupled linear equations for the bra coefficients $\widetilde{\mathsf{S}}$, with the ket state coefficients already known. It is to be noted here that the series of nested commutators in $e^{-\mathcal{S}}[H, \sigma_{\mathbf{i}_1}^+ \cdots \sigma_{\mathbf{j}_n}^+]e^{\mathcal{S}}$ terminates after a finite number of terms.

The correlation operators in the LSUB$_4$ scheme are:

$$\widetilde{S}_2 = \sum_{i,j} \left[\widetilde{a}_1 \ \sigma^-_{2i,j}\sigma^-_{2i+1,j} + \widetilde{b}_1\sigma^-_{2i,j}\sigma^-_{2i-1,j} \ + \widetilde{c}_1\sigma^-_{i,2j}\sigma^-_{i,2j+1} + \widetilde{d}_1\sigma^-_{i,2j}\sigma^-_{i,2j-1} \right]$$

$$\widetilde{S}_3 = \sum_{i,j} \left[\widetilde{a}_3\sigma^-_{2i,j}\sigma^-_{2i+3,j} \ + \widetilde{b}_3\sigma^-_{2i,j}\sigma^-_{2i-3,j} \ + \widetilde{c}_3\sigma^-_{i,2j}\sigma^-_{i,2j+3} + \widetilde{d}_3\sigma^-_{i,2j}\sigma^-_{i,2j-3} \right]$$

$$\widetilde{S}_4 = \sum_{i,j} \left[\widetilde{f} \prod_{\nu=0}^{3} \sigma^-_{2i+\nu,j} + \widetilde{g} \prod_{\nu=0}^{3} \sigma^-_{2i-\nu,j} + \widetilde{h} \prod_{\nu=0}^{3} \sigma^-_{i,2j+\nu} + \widetilde{l} \prod_{\nu=0}^{3} \sigma^-_{i,2j-\nu} \right] \qquad (22)$$

In these equations, the coefficients $\widetilde{a}_1, \widetilde{b}_1,$ etc., are various forms of the coefficient $\widetilde{S}_{\mathbf{i}_1\ldots\mathbf{i}_n \,;\, \mathbf{j}_1\ldots\mathbf{j}_n}$ in the expressions for $\widetilde{s}_{2n}$. In the LSUB$_4$ scheme, the staggered magnetization, given by

$$M^z = -\frac{2}{N} \sum_i < \sigma^z_i >,$$

where $\mathbf{i}$ runs over **o**ne sublattice only, becomes

$$M^z = 1 - \widetilde{a}_1 a_1 - \widetilde{b}_1 b_1 - \widetilde{a}_3 a_3 - \widetilde{b}_3 b_3 - 2\widetilde{f}f - 2\widetilde{g}g - \widetilde{c}_1 c_1 - \widetilde{d}_1 d_1 - \widetilde{c}_3 c_3 - \widetilde{d}_3 d_3 - 2\widetilde{h}h - 2\widetilde{l}l$$

The bra state coefficients are determined from the following set of simultaneous equations:

$$(-\tfrac{1}{2} + \widetilde{b}_1 b_1 + \widetilde{a}_1 a_1 + \widetilde{a}_3 a_3 + \widetilde{b}_3 b_3 + b_1^2\widetilde{g} + b_1 a_1\widetilde{f} + 2\widetilde{g}g + 2\widetilde{f}f)J_{x,+1}+$$
$$(\widetilde{a}_1 + \widetilde{a}_1 b_1 - \widetilde{a}_3 a_1 - 2\widetilde{f}a_1 + 2\widetilde{f}b_1 a_1 + \widetilde{f}a_3 b_3 + \tfrac{1}{2}\widetilde{g}b_3 b_1)J_{x,-1} = 0$$

$$(\widetilde{b}_1 + \widetilde{b}_1 a_1 - \widetilde{b}_3 b_1 - 2\widetilde{g}b_1 + 2\widetilde{g}b_1 a_1 + \widetilde{g}b_3 a_3 + \tfrac{1}{2}\widetilde{f}a_1 a_3)J_{x,+1}+$$
$$(-\tfrac{1}{2} + \widetilde{a}_1 a_1 + \widetilde{b}_1 b_1 + \widetilde{a}_3 a_3 + \widetilde{b}_3 b_3 + \widetilde{f}a_1^2 + \widetilde{g}b_1 a_1 + 2\widetilde{f}f + 2\widetilde{g}g)J_{x,-1} = 0$$

$$(-\widetilde{a}_1 b_1 - \widetilde{b}_1 b_3 + \widetilde{a}_3 + \widetilde{a}_3 a_1 - 2\widetilde{f}b_1 + \widetilde{f}b_1^2 - \widetilde{f}b_1 a_1 + \widetilde{g}b_1 b_3)J_{x,+1}+$$
$$(-\widetilde{a}_1 b_3 + \widetilde{a}_3 + \widetilde{a}_3 b_1 + \widetilde{f}b_3 a_1 + 2\widetilde{f}g)J_{x,-1} = 0$$

$$(-\widetilde{b}_1 a_3 + \widetilde{b}_3 + \widetilde{b}_3 a_1 + \widetilde{g}b_1 a_3 + 2\widetilde{g}f)J_{x,+1}+$$
$$(-\widetilde{b}_1 a_1 - \widetilde{a}_1 a_3 + \widetilde{b}_3 + \widetilde{b}_3 b_1 - 2\widetilde{g}a_1 + \widetilde{g}a_1^2 - \widetilde{g}b_1 a_1 + \widetilde{f}a_1 a_3)J_{x,-1} = 0$$

$$(-\widetilde{a}_1 + 2\widetilde{f}a_1 + \widetilde{g}b_3)J_{x,+1} + (-\tfrac{1}{2}\widetilde{a}_1 + \widetilde{f} + 2\widetilde{f}b_1)J_{x,-1} = 0$$

$$(-\tfrac{1}{2}\widetilde{b}_1 + \widetilde{g} + 2\widetilde{g}a_1)J_{x,+1} + (-\widetilde{b}_1 + 2\widetilde{g}b_1 + \widetilde{f}a_3)J_{x,-1} = 0$$

$$(-\tfrac{1}{2} + \widetilde{d}_1 d_1 + \widetilde{c}_1 c_1 + \widetilde{c}_3 c_3 + \widetilde{d}_3 d_3 + d_1^2\widetilde{l} + d_1 c_1\widetilde{h} + 2\widetilde{l}l + 2\widetilde{h}h)J_{y,+1}+$$
$$(\widetilde{c}_1 + \widetilde{c}_1 d_1 - \widetilde{c}_3 c_1 - 2\widetilde{h}c_1 + 2\widetilde{h}d_1 c_1 + \widetilde{h}c_3 d_3 + \tfrac{1}{2}\widetilde{l}d_3 d_1)J_{y,-1} = 0$$

$$(\widetilde{d}_1 + \widetilde{d}_1 c_1 - \widetilde{d}_3 d_1 - 2\widetilde{l}d_1 + 2\widetilde{l}d_1 c_1 + \widetilde{l}d_3 c_3 + \tfrac{1}{2}\widetilde{h}c_1 c_3)J_{y,+1}+$$
$$(-\tfrac{1}{2} + \widetilde{c}_1 c_1 + \widetilde{d}_1 d_1 + \widetilde{c}_3 c_3 + \widetilde{d}_3 d_3 + \widetilde{h}c_1^2 + \widetilde{l}d_1 c_1 + 2\widetilde{h}h + 2\widetilde{l}l)J_{y,-1} = 0$$

$$(-\widetilde{c}_1 d_1 - \widetilde{d}_1 d_3 + \widetilde{c}_3 + \widetilde{c}_3 c_1 - 2\widetilde{h}d_1 + \widetilde{h}d_1^2 - \widetilde{h}d_1 c_1 + \widetilde{l}d_1 d_3)J_{y,+1}+$$
$$(-\widetilde{c}_1 d_3 + \widetilde{c}_3 + \widetilde{c}_3 d_1 + \widetilde{h}d_3 c_1 + 2\widetilde{h}l)J_{y,-1} = 0$$

$$(-\widetilde{d}_1 c_3 + \widetilde{d}_3 + \widetilde{d}_3 c_1 + \widetilde{l}d_1 c_3 + 2\widetilde{l}h)J_{y,+1}+$$
$$(-\widetilde{d}_1 c_1 - \widetilde{c}_1 c_3 + \widetilde{d}_3 + \widetilde{d}_3 d_1 - 2\widetilde{l}c_1 + \widetilde{l}c_1^2 - \widetilde{l}d_1 c_1 + \widetilde{h}c_1 c_3)J_{y,-1} = 0$$

$$(-\widetilde{c}_1 + 2\widetilde{h}c_1 + \widetilde{l}d_3)J_{y,+1} + (-\tfrac{1}{2}\widetilde{c}_1 + \widetilde{h} + 2\widetilde{h}d_1)J_{y,-1} = 0$$

$$(-\tfrac{1}{2}\widetilde{d}_1 + \widetilde{l} + 2\widetilde{l}c_1)J_{y,+1} + (-\widetilde{d}_1 + 2\widetilde{l}d_1 + \widetilde{h}c_3)J_{y,-1} = 0$$

7

III. RESULTS

The ground state energy and magnetization can now be calculated as functions of the dimerization parameter δ. Previous calculations have invariably taken spin-spin exchange couplings alternately as $J(1 \pm \delta)$, which, as mentioned above, can be taken as an expansion of the interaction in Eq.(2) to order δ, implying that the results are valid only in the critical regime $\delta \to 0$. We notice in our calculations that if in Eqs.(2-6) all the expansions are terminated at the order of δ then the distinction between configurations (a) and (b) disappears. On the other hand, if the expansion is taken to one order higher, then there remains no way to distinguish between configurations (c) and (d). We must therefore either go to orders beyond δ^2 in the expansion, or retain the interactions in their unexpanded form. We do the latter. An added advantage is that the results will then be valid in the limit $\delta \to 1$.

A. Magnetic energy gain

Our calculations confirm that, like the chain, the ground state energy of all the five configurations decreases with δ. This is shown in Figures 2, where $\varepsilon(\delta) - \varepsilon(0)$ is plotted against δ for the proposed configurations. This conclusion is not new for some of the configurations in Fig.1 [12,18,23–26]. However, what is significant is that the ground state energy goes down with δ more rapidly for some configurations than others. In fact, Fig. 2 shows that the δ-dependence is markedly different for the two types of dimerized configurations: one in which dimerization takes place only along one axis, and the other, in which it occurs along both the directions. The rate of decrease is significantly higher for the latter. Also, the columnar configurations lead to a greater gain in magnetic energy than the staggered ones. It also shows that the plaquette configuration of Fig.1(c) is energetically the most favourable state, as also noted earlier [12,27]. Particularly in the complete range of δ ($0 \leq \delta < 1$), the plaquette configuration stands out as the most preferred one, while there is hardly a discernible difference among the configurations (a), (b) and (d).

Configuration (e) is peculiar in the sense that $\delta = \frac{1}{2}$ is a special point for it; the shorter bond length is symmetric about this point, having a minimum value of $\frac{1}{\sqrt{2}}$. At this point the distortions give rise to a rectangular lattice with sides $\sqrt{2}$ and $\frac{1}{\sqrt{2}}$. The energy gain increases with δ up to $\delta = \frac{1}{2}$, and then goes down.

It is worth pointing out here that the much simpler mean field methods of spin wave theory - either in the bosonic representation through Holstein-Primakoff transformations, or in the fermionic representation through Jordan-Wigner transformations - yield very similar results. This has been checked by us separately.

Earlier calculations on the spin-Peierls instability in a 2D system gave varied results on the critical exponents. Monte Carlo calculations of Tang and Hirsch [12] on the Hubbard model in the limit of infinite on-site repulsion U found for the cases corresponding to our configurations (a), (b), (c) and (e) that the magnetic energy gain followed a simple power law behaviour and increased as δ^2. Their cases are different from ours in the sense that couplings alternated as $J(1 \pm \delta)$, and were taken constant along the y-direction in the case (b). Feiguin et al [18] obtained similar results for configurations (a) and (e) in the Schwinger boson representation. Quantum Monte Carlo calculations of Katoh and Imada [26] showed that in chains that are coupled by an antiferromagnetic coupling the exponent of the magnetic energy gain in the $\delta \to 0$ limit is 1.

Our results are expected to be different from these because instead of $J(1 \pm \delta)$, we take the unapproximated exchange coupling $J(a) = \frac{J}{a}$. Our CCM calculations show that the gain in magnetic energy does not vary with δ as a simple power law; it varies as $\frac{\delta^v}{|\ln \delta|}$ for all the five configurations in the range $0 \leq \delta \leq 0.1$ with the exponent $\nu = 1.5$. In the complete range $0 \leq \delta < 1$ also, they show the same dependence on δ with $\nu = 1$ for the configurations (a) - (d).

It is interesting to note that earlier results show, as summarized in Table 1, that the dimerization of an antiferromagnetic chain also varies as $\frac{\delta^v}{|\ln \delta|}$, but only in the small δ regime (the near critical regime). There, the factor of $\frac{1}{|\ln \delta|}$ is brought about in the renormalization group calculations as a correction due to umklapp processes [7,28]. Our CCM results, however, show that even in chains this may be the case when the exchange couplings in the dimerized state are taken as $\frac{J}{1 \pm \delta}$, instead of the approximated $J(1 \pm \delta)$. We find for chains that the best fit is obtained with $\frac{\delta^v}{|\ln \delta|}$ in the entire range of δ rather than only in the range of small δ. With the full exchange couplings, the exponent for the chain comes out to be $\nu = \frac{2}{3}$ for $0 \leq \delta < 1$, and $\nu = 1.3$ - 1.6 for $0 \leq \delta \leq 0.1$. The latter gives a decent comparison

with the numbers in Table 1.

B. The gap parameter

The δ dependence of the energy gap parameter $D(\delta)$ defined above for the five configurations is shown in Fig.3, showing greater stabilization of the dimerized state with increasing δ. We also find that, like the magnetic energy gain, the gap parameter D increases with δ as $\frac{\delta^v}{|\ln \delta|}$ in the small δ regime for all the five configurations with $\nu = 1.5$. The configurations (a) - (d) also have the same dependence on δ in the entire range of δ with $\nu = 1$.

The difference between the dimerization of a square lattice along only one direction (Fig. 1(a) and (b)) and along both the directions (Fig. 1(c) ,(d) and (e)) is again markedly brought out in Fig. 3. Also the columnar configurations again appear as preferred modes of dimerization over the staggered configurations for having higher values of the gap parameter in the region of small δ.

C. Staggered magnetization

Our CCM calculations in the LSUB$_4$ approximation give staggered magnetization for the un-dimerized square lattice $M(\delta = 0)$= 0.2965, within about 2% of the exact value of 0.303. As dimerization sets in, magnetization decreases in all the configurations we have chosen, as shown in Fig. 4, in agreement with the earlier results for configuration (a) [25]. This is also the case for the entire range of δ ($0 \leq \delta < 1$), except in the case of configuration (e) for which the magnetization rises again after $\delta = \frac{1}{\sqrt{2}}$.

The CCM calculations show that for all the five configurations, the magnetization also varies as $\frac{\delta^v}{|\ln \delta|}$ in the small δ regime with the exponent $\nu = 1.5$, exactly as the energy gain and the gap parameter. However in the regime $0 \leq \delta < 1$, M exhibits a simple power law dependence: $M \sim \delta^x$ with x between .65 and .75, as shown in Table 2. Configuration (e) has a distinctly different behaviour in this regime.

To summarize, we have studied the spin-Peierls dimerization of a spin-half Heisenberg antiferromagnet on a square lattice taking unapproximated exchange couplings based on the ansatz $J(a) = \frac{J}{a}$, and assuming that the spin-lattice coupling is above the threshold to affect the spin-Peierls transition. We have included different possibilities of dimerization. The ground state energy as well as staggered magnetization decrease continuously with increasing dimerization for all the proposed configurations. Of the five configurations, those with dimerization taking place simultaneously along both the principal square axes have markedly lower ground state energies and magnetization than those with dimerization along only one of the axes, in agreement with the result of Lieb and Nachtergaele [27]. Also, those with columnar dimerization have consistently lower energies than those with the staggered dimerization. The plaquette configuration stands out as the most favoured mode of dimerization. The energy gap parameter also corroborates the above conclusions. It has also been shown that the magnetic energy gain as well as the gap parameter and staggered magnetization depend upon the dimerization parameter δ as $\frac{\delta^v}{|\ln \delta|}$, at least in the $\delta \to 0$ regime, the $|\ln \delta|$ factor coming in without any considerations of umklapp processes being included.

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Figure captions

Figure 1: Five configurations for the dimerization of a square lattice. (a) a columnar configuration caused by a longitudinal $(\pi, 0)$ static phonon. The nearest neighbour coupling along the horizontal direction alternates between $J(1 - \delta)$ and $J(1 + \delta)$, while that along the vertical direction remains J. (b) a staggered configuration caused by a (π, π) static phonon with polarization along x-direction. Like (a), the dimerization occurs along one direction only, but the sequence of alternate couplings itself alternates along the other direction. The coupling along the vertical direction is also taken to vary with δ. (c) Dimerization along both the directions, caused by $(\pi, 0)$ and $(0, \pi)$ phonons, making a plaquette of four nearest neighbour spins. (d) Again dimerization along both the directions, but taken staggered along the vertical direction. (e) Another staggered dimerization that is caused by a longitudinal (π, π) phonon. Chains are formed with strong bonds. The square lattice deforms to a rectangular lattice with this mode for $\delta = 1/2$.

Figure 2: The gain in magnetic energy $\varepsilon(\delta) - \varepsilon(0)$ as dimerization sets in with increasing δ for the five configurations; (a) in the range $0 \le \delta \le 0.1$, and (b) in $0 \le \delta < 1$.

Figure 3: Dependence of the energy gap parameter D on δ for the five dimerization configurations; (a) in the range $0 \le \delta \le 0.1$, and (b) in $0 \le \delta < 1$.

Figure 4: Staggered magnetization varying with δ for the five dimerization configurations; (a) in the range $0 \le \delta \le 0.1$, and (b) in $0 \le \delta \le 1$.

Table-1 : Summary of the critical exponents for spin-Peierls transition in a Heisenberg chain determined by various methods.

Method	Interval	$\varepsilon(\delta) - \varepsilon(0)$	Exponent
Random phase app. [3]	$0 \le \delta \le 1$	δ^x	$x = 4/3$
Renormalization group [4]	$0 \le \delta \le 1$	δ^x	$x = 1.53$
2-level RG [5]	$0 \le \delta \le 1$	δ^x	$x = 1.78$
	$0.05 \le \delta \le 0.1$	$\delta^{2\nu}/|\ln(\delta)|$	$2\nu = 1.68^{+0.13}_{-0.36}$
	$0.4 \le \delta \le 0.5$	$\delta^{2\nu}/|\ln(\delta)|$	$2\nu = 1.31 \pm 0.02$
Excitation spectrum [6]	$0 \le \delta \le 1$	δ^x	$x = 1.36^{+0.1}_{-0.2}$
Valence bond [7]	$\delta \le 0.05$	$\delta^{2\nu}/|\ln(\delta)|$	$\nu = 2/3$
	$\delta \ge 0.05$	δ^x	$x = 1.36^{+0.1}_{-0.2}$
Finit size scaling [8]	$0 \le \delta \le 0.1$	$\delta^{2\nu}/|\ln(\delta)|$	$\nu = 0.71 \pm 0.01$
	$0 \le \delta \le 1$	δ^x	$x = 1.34 \pm 0.02$
Exact diagonalization [9]	$0 \le \delta \le 0.1$	$\delta^{2\nu}/|\ln(\delta)|$	$\nu = 2/3$
DMRG [10]	$\delta \le 0.05$	δ^x	$x = 2/3$

Table 2: Exponents obtained by the CCM method for magnetic energy gain, energy gap and magnetization for the five dimerized square lattice configurations. The logarithmic power law goes as $\delta^{\nu}/|\ln(\delta)|$ in the five configurations for both energy gain and gap parameter for both small and full δ. While in the staggered magnetization the logarithmic law is valid for $\delta \to 0$, but it obeys a simple power law in the full dimerization limit; $\delta \to 1$. Values of ν are listed in the following table.

Configuration	Interval	$\varepsilon(\delta) - \varepsilon(0)$	$\Delta(\delta) - \Delta(0)$	$M(0) - M(\delta)$
(a)	$0 \le \delta \le 0.1$	$\nu = 1.5$	$\nu = 1.5$	$\nu = 1.5$
	$0 \le \delta < 1$	$\nu = 1.0$	$\nu = 1.0$	$\sim \delta^{0.65}$
(b)	$0 \le \delta \le 0.1$	$\nu = 1.5$	$\nu = 1.5$	$\nu = 1.5$
	$0 \le \delta < 1$	$\nu = 1.0$	$\nu = 1.0$	$\sim \delta^{0.75}$
(c)	$0 \le \delta \le 0.1$	$\nu = 1.5$	$\nu = 1.5$	$\nu = 1.5$
	$0 \le \delta < 1$	$\nu = 1.0$	$\nu = 1.0$	$\sim \delta^{0.75}$
(d)	$0 \le \delta \le 0.1$	$\nu = 1.5$	$\nu = 1.5$	$\nu = 1.5$
	$0 \le \delta < 1$	$\nu = 1.0$	$\nu = 1.0$	$\sim \delta^{0.65}$
(e)	$0 \le \delta \le 0.1$	$\nu = 1.5$	$\nu = 1.5$	$\nu = 1.5$
	$0 \le \delta < 1$			$\sim \delta^{0.1}$